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ATOMISTIC AND FE MODELLING OF CRYSTAL LATTICE DEFECTS EXAMINED BY HRTEM

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ABSTRACT

Many of crystal defects like dislocations and interfacial structures formed between two quite different crystallographic structures result the residual stresses and coupled physical fields being the crucial for understanding the conditions of crystal growth. The next question is why in some cases the growth results the flat layers while in others the channels, quantum dots or nanowires form. Such complex technological problems of crystal growth compose a quite new challenge for the computer modelling.

In the preset paper we consider the atomic nets with dislocations and interfacial layer embedded in a 3D finite element mesh. Thanks to such a multiscale approach the physical tensor fields like residual stresses, electric field, and the gradients of chemical and electronic concentrations sharing the atomistic model can be considered simultaneously in terms of FE method and atomistic models.

In the first example we consider the GaN/AlN Quantum Dots (QDs) nucleating at the edge of threading dislocations (TDs). This phenomenon was observed experimentally first by Rouviere et al. [1]. It was caused by the fact that TDs induce local tension regions of crystal lattice. This, in turn, gives the geometric condition for nucleation of the QDs with a larger lattice spacing than these in relaxed substrate.

Concerning the FE part, as an example, we consider the inelastic flow induced by residual stresses and chemical potential force in semiconductor layers. The constitutive equations for plastic flow are based on the transport of chemical components induces by the gradient of residual stresses [GPa/nm] and chemical potential in semiconductor layers [2]. The previous thermodynamic model and 3D FE simulation was shown [3].

Concerning the atomistic part, we present a 3D atomic net of a system composed of QDs situated on the edges of threading dislocations. The resultant chemical segregation obtained from our FE simulation is next reconstructed in the atomistic level.

The computational scheme employed here allows to use two independent computational tools, namely the continuous model in which we consider the physical tensor fields and the second, atomistic tool into which the data from the resultant FE calculation can be translated. Such obtained atomistic model can be used next in many atomic (discrete) level methods like MD, Monte Carlo or ab-initio method.

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